



**INFORMATION ONLY**

**OFFICE OF SCIENCE & TECHNOLOGY AND INTERNATIONAL**

**Technical Work Plan for:**

**ENHANCED RETARDATION OF RADIONUCLIDE  
TRANSPORT IN FRACTURED ROCK**

**OSTI-LBNL-TWP-000001, REV 00 ICN 01**

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**CHANGE HISTORY**

| <b>Revision<br/>Number</b> | <b>ICN<br/>Number</b> | <b>Date of<br/>Change</b> | <b>Description of Change</b>          |
|----------------------------|-----------------------|---------------------------|---------------------------------------|
| 00                         | 00                    | 06/30/04                  | Initial issue.                        |
| 00                         | 01                    | 10/29/04                  | Modification to update the TWP title. |

## ACRONYMS

|       |  |
|-------|--|
| COTS  | Commercial off the Shelf Software                |
| DOE   | Department of Energy                             |
| FY    | Fiscal Year                                      |
| ICN   | Interim Change Notice                            |
| LA    | License Application                              |
| LBNL  | Lawrence Berkeley National Laboratory            |
| NRC   | Nuclear Regulatory Commission                    |
| OCRWM | Office of Civilian Radioactive Waste Management  |
| OSTI  | Office of Science & Technology and International |
| PI    | Principal Investigator                           |
| PM    | Project Manager                                  |
| QA    | Quality Assurance                                |
| QARD  | Quality Assurance Requirements and Description   |
| QIP   | Quality Implementing Procedure                   |
| SCM   | Software Configuration Management                |
| SZ    | Saturated Zone                                   |
| TDMS  | Technical Data Management System                 |
| TSPA  | Total System Performance Assessment              |
| TWP   | Technical Work Plan                              |

UZ                      Unsaturated Zone

YMP                    Yucca Mountain Project

## 1. SCOPE

This Technical Work Plan (TWP) supports the scientific investigation activities performed for the US Department of Energy (DOE) Office of Science & Technology and International (OSTI) by the Lawrence Berkeley National Laboratory (LBNL). The purpose of the planned scientific investigation is to improve our understanding of the field-scale matrix diffusion processes and to acquire the data that may lead to improved potential performance of the unsaturated zone (UZ) as a barrier.

This TWP describes work to be performed in further analyzing the function of the UZ serving as one of the natural barriers to the transport of radionuclides within the proposed High-Level Radioactive Waste Repository at Yucca Mountain. The UZ acts as a natural barrier by retarding the flow of infiltrating water and radionuclide transport downward toward the water table; by facilitating contact with sorbing minerals for any radionuclides that are released into the UZ; by sequestering contaminated fluids in the rock matrix or low-flow zones; and by channeling flow in zones away from the repository block. The repository is designed to take advantage of these attributes by placing the waste in drifts well above the water table and away from significant fault zones.

These studies will address the scale dependency of effective matrix diffusion coefficients through an extensive survey of existing estimates at Yucca Mountain, plus sites elsewhere in the world. The effective matrix diffusion coefficient is an important parameter for describing matrix diffusion, and its magnitude largely determines overall radionuclide transport behavior in fractured rock. The theoretical basis for scale dependency will be established through modeling and data collected in the supporting studies and experiments. Finally, the effect of scale dependency on radionuclide transport will be documented through flow and transport modeling.

This work is governed by the Guidance and Funds to Lawrence Berkeley National Laboratory for Tasks from the Office of Civilian Radioactive Waste Management Memorandum, dated 1/20/04. Annual progress reports will be submitted to DOE by September 30, 2004, 2005 and an interpretive report by September 30, 2006.

### 1.1 OBJECTIVES

The effectiveness of the natural UZ barrier depends both on its ability to retard water flow and radionuclide transport through fracture-matrix interactions, and to enhance the sorption of released radionuclides on rock surfaces, such as fractures within the drift wall or pore surfaces within the bedded tuff. The degree of radionuclide retardation and/or sorption will largely depend on the degree of fracture-matrix interactions including matrix diffusion. Studies that enhance our understanding of these interactions will permit modelers to reduce the uncertainty in estimates of radionuclide transport, and to develop more realistic estimates of the accompanying dose rates.

Matrix diffusion coefficient values measured from small rock samples in the laboratory have been used for modeling radionuclide transport at the Yucca Mountain site. Most recently, Liu et al. (2004) pointed out, for the first time, that the effective matrix diffusion coefficient for field-scale problems might be scale-dependent and increases with test scale. The main objective of this

study is to improve our understanding of effects of matrix diffusion on retardation of Radionuclide Transport in Fractured Rock. This will be accomplished by (1) further evaluating the scale-dependent behavior of the effective matrix diffusion coefficient, (2) developing a rigorous theoretical basis of the scale dependency, and (3) demonstrating the conservatism in estimated natural-system performance at the Yucca Mountain Site (when the scale dependency is not considered).

## **1.2 PRIMARY TASKS**

### **1.2.1 Confirmation of the Scale-Dependent Behavior of the Effective Matrix Diffusion Coefficient**

This task consists of three activities.

- A. A comprehensive survey of estimates of the effective matrix diffusion coefficient published in the literature will be conducted. A clear relation between the effective diffusion coefficient and test scale will be defined.
- B. Selected tracer-test results in the literature will be reanalyzed to evaluate the values for the effective diffusion coefficient reported by other researchers and to provide additional evidence for the scale dependency. In particular, data sets involving tracer-test results at different scales (or results observed at locations with different distances from the tracer release point for a given site) will be analyzed to show the potential scale dependency at a given test site. Mass transfer coefficient data from dual porosity studies in highly heterogeneous soils and sediments will also be analyzed as the corroborative evidence.
- C.  $C^{14}$  data (and other geochemical data) have been collected from the Yucca Mountain site and used as an indicator of water travel times. Simulation results will be compared with these data sets to check for the consistency between the data and the potential scale-dependent behavior.

### **1.2.2 Development of a Theoretical Basis for the Scale Dependency**

While the scale dependency of permeability and dispersivity has been known for many years, the scale dependency of the matrix-diffusion coefficient is a completely new research topic. The mechanisms behind this surprising scale-dependency behavior are not clear. Liu et al. (2004) offered a preliminary explanation based on the hypothesis that solute travel paths within a fracture network are fractals. The focus of this task is on full development of a theoretical basis for the scale dependency based on the work of Liu et al. (2004). Two-dimensional fracture-network models (with matrix) will be used to perform numerical experiments. Previous studies have shown that both fracture roughness and fracture networks are fractals (Liu et al. 2004). The capabilities for computationally generating fracture networks characterized by fractal geometry will be developed as a part of this task. Detailed numerical simulations of flow and tracer transport through fracture networks (including the matrix) will be performed to generate tracer breakthrough curves as a function of test scale. Effective matrix-diffusion-coefficient values will be estimated from the simulated breakthrough curves. From these numerical experiment results, a theoretical basis will be developed for a potential relationship between the effective coefficient values and the test scale.

If the results of the numerical experiments were to contradict the explanation of Liu et al. (2004), then alternative explanations will be explored and developed.

### **1.2.3 Demonstration of the Conservatism of the Natural-System Performance Calculated without Considering the Scale Dependency of the Effective Matrix Diffusion Coefficient**

The Yucca Mountain UZ site-scale flow and transport models will be used for simulating radionuclide transport. Simulation results with and without considering the scale dependency of the effective matrix-diffusion coefficient will be compared for different scenarios. Special attention will be given to the scenarios used by Total System Performance Assessment (TSPA) for License Application (LA).

## **1.3 ACCURACY, PRECISION, AND REPRESENTATIVENESS OF RESULTS.**

The accuracy, precision, and representativeness of the results of the model, and how these were determined will be addressed in any technical or model reports generated as part of these activities. Uncertainties associated with the models are a function of the specific application, and should be determined by the use of model specific validation test cases.

Numerical representation of a real world system involves discretization of a model volume into a large number of elements, with each element assigned the necessary attributes or properties. For large models, such as the UZ model, the necessary attributes or properties are known at only few locations within the model domain. Errors may result during numerical grid development from the simplification of the infinitely complex natural system into a final set of (fairly coarse) elements, from erroneous conceptualization of a physical system, or inaccuracy in describing physical processes. Limitations of the software used to develop numerical grids of the UZ Model may also create a potential source of error that is addressed in the Software Qualification per the Quality Implementing Procedure (QIP), OSTI-LBNL-QIP-SI.0, *Software Management*.

## **2. SCIENTIFIC APPROACH OR TECHNICAL METHODS**

This section establishes the implementation plan and work controls to perform the primary tasks.

### **2.1 WORK ACTIVITIES**

- A. Confirmation of the scale-dependent behavior of the effective matrix-diffusion coefficient: Fiscal Years (FY) 2004 and 2005;
- B. Development of a theoretical explanation for the scale dependency: FY 2004 and 2005;
- C. Demonstration of the conservatism of the natural-system performance calculated without considering the scale dependency of the effective matrix diffusion coefficient: FY 2006.

#### **2.1.1 Responsible Organizations**

The OSTI-LBNL Project Manager (PM) shall have the overall responsibility for the execution of the work identified in this plan along with applicable OSTI-LBNL Principal Investigator (PI),

technical personnel, and subcontractors working under the OSTI-LBNL TWP and Quality Assurance (QA) program.

### **2.1.2 Intended Use of Products**

The planned study has the potential to demonstrate that the performance of natural systems at Yucca Mountain has been significantly underestimated by the Yucca Mountain Project (YMP). Results from this proposed work will increase confidence in repository performance and enhance scientific defensibility of TSPA for LA. This study also has the potential to open up a new research area that is critical not only for the Yucca Mountain site, but also for the other geological disposal sites (fractured porous media) under consideration worldwide. Therefore, the research is important for maintaining U.S. scientific leadership in nuclear waste management and for increasing acceptance of Yucca Mountain as a suitable site by both the public and the scientific community

The research results will be published in report(s) and in peer-reviewed journals as described in the Guidance and Funds to Lawrence Berkeley National Laboratory for Tasks from the Office of Civilian Radioactive Waste Management Memorandum, dated 1/20/04 for Fiscal Year 2004.

### **2.1.3 Scientific Approach and Technical Methods**

Owing to the order-of-magnitude slower flow velocity in the matrix compared to fractures, matrix diffusion can significantly retard radionuclide transport in fractured rock. The effective matrix diffusion coefficient is an important parameter for describing matrix diffusion, and its magnitude largely determines overall radionuclide transport behavior in fractured rock. Matrix diffusion coefficient values measured from small rock samples in the laboratory have been used for modeling radionuclide transport at the Yucca Mountain site. Most recently, Liu et al. (2004) pointed out that the effective matrix diffusion coefficient for field-scale problems might be scale-dependent.

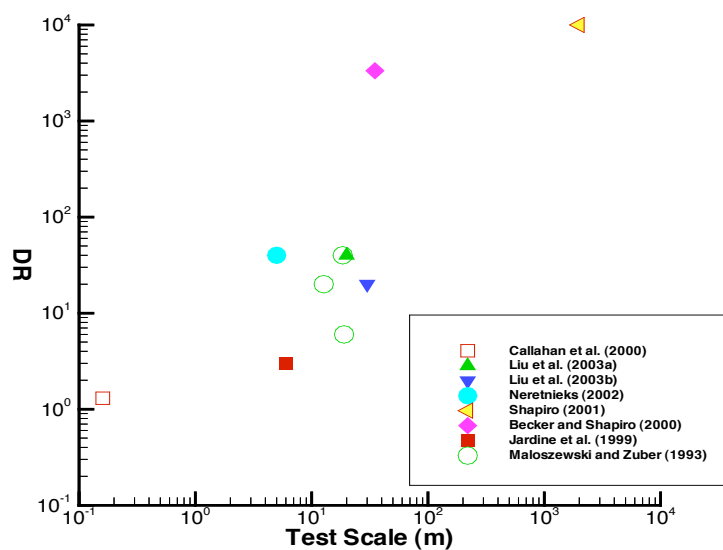


Figure 1. Effective matrix diffusion coefficient as a function of test scale (Liu et al., 2004). *RD* refers to the effective coefficient value (estimated from field data) divided by the corresponding local value.

If the preliminary finding of Liu et al. (2004) proves to be true, the matrix-diffusion-coefficient values currently used by the YMP are expected to be several orders of magnitude smaller than actual values, as suggested by Figure 1. (Note that the “test scale” for the Yucca Mountain site, or the length of a flow path from the repository to the assessable environment, is on the order of  $10^3$  meters.) In other words, the performance of natural systems [including both UZ and Saturated Zone (SZ)] may have been significantly underestimated.

In order to confirm this potentially important finding and to understand the physical mechanisms behind this scale-dependent behavior, we take the following approach. literature survey of estimates of the effective matrix diffusion coefficient, reanalysis of selected tracer test results in the literature, and comparisons between simulation results and the selected data from the Yucca Mountain site will be performed to confirm the scale-dependent behavior. Mass transfer coefficient data from dual porosity studies in highly heterogeneous soils and sediments will also be analyzed as the corroborative evidence. Two dimensional, detailed fracture-network models (with matrix) will be used to perform numerical experiments to develop a rigorous theoretical basis for the scale dependency. New software for generating fractal fracture networks and solute transport through them will be developed. The site-scale unsaturated zone flow and transport models will be used for simulating radionuclide transport. Simulation results with and without considering the scale dependency of the effective matrix-diffusion coefficient will be compared for different scenarios. Special attention will be given to the scenarios used by TSPA for LA.

#### 2.1.4 Data Collection, Reduction and Recording Methodology

No new data will be collected in association with these activities.

### 2.1.5 Unexpected Test Results, Test Conditions, or Off-Normal Event Occurrence During Testing

There is no testing associated with these analyses.

## 2.2 ADDITIONAL MODELING AND SCIENTIFIC ANALYSIS ACTIVITIES

N/A. Preliminary modeling activities will be conducted as part of this TWP and the results will be presented in report(s) and in peer-reviewed journals as described in the Guidance and Funds to Lawrence Berkeley National Laboratory for Tasks from the Office of Civilian Radioactive Waste Management Memorandum, dated 1/20/04 for Fiscal Year 2004.

## 3. INDUSTRY STANDARDS, FEDERAL REGULATIONS, DOE ORDERS, REQUIREMENTS, AND ACCEPTANCE/COMPLETION CRITERIA

This work is governed by the Guidance and Funds to Lawrence Berkeley National Laboratory for Tasks from the Office of Civilian Radioactive Waste Management Memorandum, dated 1/20/04 for Fiscal Year 2004.

## 4. IMPLEMENTING DOCUMENTS

Even though this work is expected to be preliminary, the following procedures, as appropriate, will be used to perform the work. The most recent applicable procedures will be used.

Table 1. OSTI-LBNL Implementing Procedures

|                   |  |
|-------------------|--|
| OSTI-LBNL-QIP-1.0 | <i>OSTI-LBNL Organizational Structure</i>  |
| OSTI-LBNL-QIP-2.0 | <i>Indoctrination and Training of Personnel</i>  |
| OSTI-LBNL-QIP-2.1 | <i>Establishment and Verification of Required Education and Experience of Personnel</i>  |
| OSTI-LBNL-QIP-2.2 | <i>Planning for Science Activities</i>   |
| OSTI-LBNL-QIP-2.3 | <i>Surveillances</i>   |
| OSTI-LBNL-QIP-4.0 | <i>Procurement Document Control</i>  |
| OSTI-LBNL-QIP-5.0 | <i>Preparing the Quality Assurance Plan and Quality/Technical Implementing Procedure</i> |
| OSTI-LBNL-QIP-6.0 | <i>Controlled Documents</i>  |
| OSTI-LBNL-QIP-6.1 | <i>Document Review</i>   |

|                       |  |
|-----------------------|--|
| OSTI-LBNL-QIP-7.0     | <i>Control of Purchased Services</i>   |
| OSTI-LBNL-QIP-16.0    | <i>Condition Reporting and Resolution</i>  |
| OSTI-LBNL-QIP-17.0    | <i>Records Management</i>  |
| OSTI-LBNL-QIP-18.0    | <i>Quality Assurance Audits and Management Assessments</i>                         |
| OSTI-LBNL-QIP-SI.0    | <i>Software Management</i>   |
| OSTI-LBNL-QIP-SIII.0  | <i>Scientific Notebooks</i>  |
| OSTI-LBNL-QIP-SIII.1* | <i>Technical Reports</i>   |
| OSTI-LBNL-QIP-SIII.2* | <i>Model Reports</i>   |
| OSTI-LBNL-QIP- SIII.3 | <i>Submittal and Incorporation of Data to the Technical Data Management System</i> |
| OSTI-LBNL-QIP- SIII.4 | <i>Qualification of Unqualified Data</i>   |
| OSTI-LBNL-QIP-SV.0    | <i>Management of OSTI-LBNL Electronic Data</i>                                     |

\* To be invoked by management direction

## 5. EQUIPMENT

The annual progress reports will be prepared using project standard desktop computers. No field or laboratory work will be conducted as part of this plan. No calibration or other test equipment will be used.

## 6. RECORDS

Records generated, as a result of implementing procedures listed in Section 4, will be collected and submitted in accordance with OSTI-LBNL-QIP-17.0.

## 7. QUALITY VERIFICATIONS

No quality assurance verifications, other than regularly scheduled audits and surveillances, are required during the execution of this TWP.

## 8. PRE-REQUISITES, SPECIAL CONTROLS, ENVIRONMENTAL CONDITIONS, PROCESSES, OR SKILLS

The work will be performed in accordance with the DOE Office of Civilian Radioactive Waste Management (OCRWM) *Quality Assurance Requirements and Description (QARD)*, DOE/RW-0333P.

## 8.1 PREREQUISITES

Data that are to be used as input for the reports shall be submitted to the Technical Data Management System (TDMS) in accordance with OSTI-LBNL-QIP-SIII.3.

## 8.2 SUPPLEMENT V APPLICABILITY

For the work conducted by OSTI-LBNL technical staff and subcontractors, the electronic management of information will be controlled under the OSTI-LBNL-QIP-SV.0.

## 8.3 ENVIRONMENTAL CONTROLS

The scientific investigation described within this TWP will be performed at LBNL and the Clemson University Campus in South Carolina. Special environmental conditions are not required for this work. No radioactive materials will be used in this work.

## 8.4 QUALIFICATION REQUIREMENTS

Training requirements for the OSTI-LBNL personnel and subcontractors working under the OSTI-LBNL QA Program will be established in the OSTI-LBNL training matrix. Compliance with the training requirements will be evaluated by OSTI-LBNL QA Manager (or designee) through a review of completed training records. The qualifications of originators and reviewers of reports will be verified in accordance with OSTI-LBNL-QIP-2.1.

## 9. SOFTWARE

Software used for performing numerical simulations will be developed in accordance with OSTI-LBNL-QIP-SI.0 or requested from the YMP SCM if previously qualified in accordance with applicable YMP procedures (see Table 2 for a list of YMP qualified software.)

New software will be developed in this study (Section 2.1.3). Software may be used prior to qualification to develop a preliminary output. The preliminary output will be documented and controlled in accordance with OSTI-LBNL-QIP-SIII.3. The final output shall be produced with baselined software in accordance with OSTI-LBNL-QIP-SI.0.

Data reductions, spreadsheets, and graphic presentation of data using commercial off-the-shelf software (COTS) programs (e.g., Microsoft Excel) may be used to synthesize, summarize, or graphically present data. The computation shall be documented such that the results can be independently reproduced or checked by hand. This software use is considered exempt from the requirements of OSTI-LBNL-QIP-SI.0 provided that adequate information is included in the scientific notebook or the report using this software.

Table 2. Qualified Software

| Software Name | Version | Software Tracking Number |
|---------------|---------|--------------------------|
| INFIL2GRID    | 1.7     | 10077-1.7-00             |
| T2R3D         | 1.4     | 10006-1.4-00             |
| TOUGH2        | 1.4     | 10007-1.4-01             |

Continuous use software, such as that used for data collection, is not planned in this report.

## **10. ORGANIZATIONAL INTERFACES**

DOE OSTI personnel will review the annual reports and provide input, as appropriate. The Clemson University personnel will work under the OSTI-LBNL QA Program and technical guidance of the OSTI-LBNL Principal Investigator (PI) as specified in the procurement documents.

The DOE Office of Quality Assurance will conduct audits of the OSTI-LBNL activities as described in OSTI-LBNL-QIP-18.0.

## **11. PROCUREMENT**

The types of subcontractor services required for the activities identified in this plan include analytical services for the scientific analysis activities conducted using computers in office environments.

## **12. REFERENCES**

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